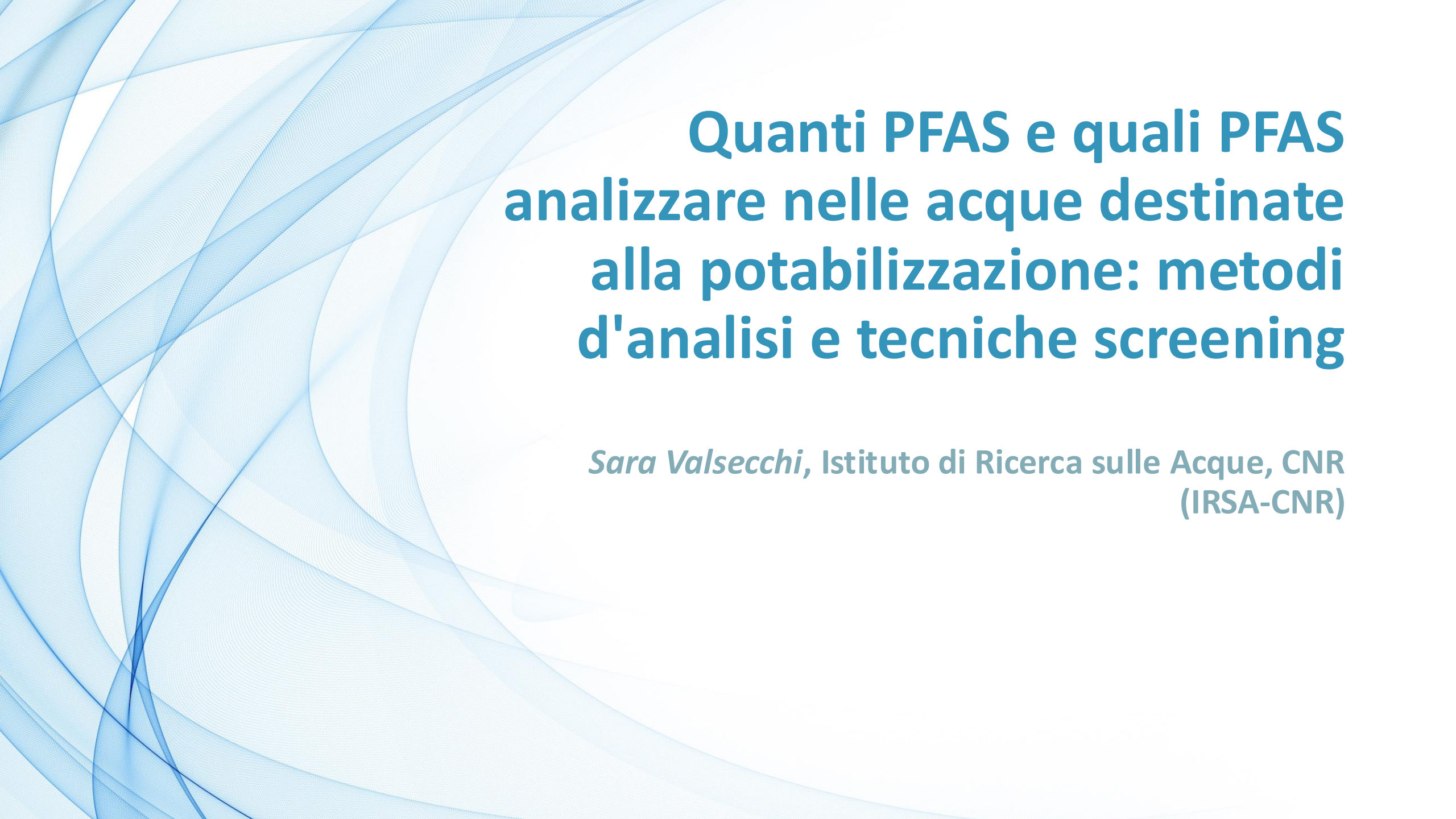




# **Quanti PFAS e quali PFAS analizzare nelle acque destinate alla potabilizzazione: metodi d'analisi e tecniche screening**

*Sara Valsecchi, Istituto di Ricerca sulle Acque, CNR  
(IRSA-CNR)*

# DIRETTIVA (UE) 2020/2184 DEL PARLAMENTO EUROPEO E DEL CONSIGLIO del 16 dicembre 2020 concernente la qualità delle acque destinate al consumo umano

Le sostanze ricomprese nel parametro «**somma di PFAS**» sono elencate nell'allegato III, parte B, punto 3, della direttiva.

- PFCA C4-C13 (PFBA-PFTrA)
- PFSA C4-C13 (PFBS-PFTrS)

|                   |             |
|-------------------|-------------|
| — «PFAS — totale» | = 0,50 µg/l |
| — «somma di PFAS» | = 0,10 µg/l |

Le sostanze che fanno parte della «**somma di PFAS**» contengono un gruppo perfluoroalchilico con tre o più atomi di carbonio (vale a dire  $-C_nF_{2n}-$ ,  $n \geq 3$ ) o un gruppo perfluoroalchil etero con due o più atomi di carbonio (vale a dire  $-C_nF_{2n}OC_mF_{2m}-$ ,  $n$  e  $m \geq 1$ ). La catena è composta in totale da 4 a 13 atomi di carbonio, il che determina 10 acidi perfluoroalchil carbossilici (PFCAs) e 10 acidi perfluoroalchil solfonici (PFSAs).

A causa della definizione data dalla direttiva, **i composti di PFAS a catena ultracorta con 2 o 3 atomi di carbonio sono esclusi dalla «somma di PFAS»**, in particolare l'acido trifluoroacetico (TFA) e l'acido perfluoropropanoico (PFPrA), così come l'acido trifluorometanosolfonico (TFMS), l'acido perfluoroetanosolfonico (PFETs) e l'acido perfluoropropanosolfonico (PFPrS).

Il parametro «**PFAS — totale**» è definito nell'allegato I della direttiva come «*la totalità delle sostanze per- e polifluoro alchiliche*».

DECRETO LEGISLATIVO 19 giugno 2025, n. 102.

**Disposizioni integrative e correttive del decreto legislativo 23 febbraio 2023, n. 18, di attuazione della direttiva (UE) 2020/2184 del Parlamento europeo e del Consiglio, del 16 dicembre 2020, concernente la qualità delle acque destinate al consumo umano.**

Art. 21.

*Modifiche all'articolo 24  
del decreto legislativo 23 febbraio 2023, n. 18*

.....le parole: «**PFAS-totale,**» sono **soppresse** e dopo le parole: «**somma di PFAS**» sono inserite le seguenti: «**, somma di 4 PFAS,**».....

|               |      |      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|---------------|------|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Somma di PFAS | 0,10 | µg/l | <p>monitoraggio.</p> <p>Per «somma di PFAS» si intende la somma di tutte le sostanze per- e polifluoroalchiliche di cui all'allegato III, Parte B, punto 3, ritenute preoccupanti per quanto riguarda le acque destinate al consumo umano.</p> <p>Nel parametro «somma di PFAS» sono da considerare PFAS supplementari non inclusi in allegato III, Parte B, punto 3, laddove rilevanti per specifiche circostanze territoriali, sulla base delle analisi di pressione per le zone di alimentazione e di ogni altra informazione disponibile. Nel caso di attività produttive che possono costituire potenziali fonti di contaminazione delle acque e che siano associate a produzione o impiego rilevante di PFAS non inclusi nell'allegato III, Parte B punto 3, per i quali non sono disponibili standard analitici, si raccomanda alla competente autorità incaricata delle procedure</p> |
|---------------|------|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

|  |  |  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|--|--|--|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|  |  |  | <p>autorizzative ambientali, di prescrivere al gestore dell'attività produttiva il conferimento di una adeguata quantità di sostanza pura da utilizzare per le attività analitiche associate ai controlli esterni di cui all'articolo 13.</p> <p>L'Autorità sanitaria locale preposta al controllo della qualità delle acque destinate al consumo umano, sentita l'autorità sanitaria regionale e l'ISS, può adottare valori più restrittivi in specifiche circostanze territoriali, tenuto conto in particolare dell'esposizione pregressa alle sostanze per- e polifluoroalchiliche della popolazione interessata.</p> |
|--|--|--|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

|                 |      |      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|-----------------|------|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Somma di 4 PFAS | 0,02 | µg/l | <p>Per «somma di 4 PFAS» si intende la somma delle seguenti sostanze: acido perfluorooctanoico (PFOA), acido perfluorooctansolfonico (PFOS), acido perfluorononanoico (PFNA) e acido perfluoroesano solfonico (PFHxS). Si tratta di un sottoinsieme di sostanze incluse nel parametro "somma di PFAS".</p> <p>L'Autorità sanitaria locale preposta al controllo della qualità delle acque destinate al consumo umano, sentita l'autorità sanitaria regionale e l'Istituto superiore di sanità, può adottare valori più restrittivi in specifiche circostanze territoriali, tenuto conto in particolare dell'esposizione pregressa alle sostanze per- e polifluoroalchiliche della popolazione interessata.</p> |
|-----------------|------|------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

|                        |    |      |  |
|------------------------|----|------|--|
| Acido trifluoroacetico | 10 | µg/l |  |
|------------------------|----|------|--|

## PFCA C4-C13 (PFBA-PFTrA)

## PFSA C4-C13 (PFBS-PFTrS)

- acido 2,3,3,3-tetrafluoro-2-(eptafluoropropossi)propanoico (HFPO-DA o GenX)
- acido dodecafluoro-3H-4,8-diossanonanoico (ADONA)
- fluorotelomero solfonato (6:2 FTS)
- acido difluoro{[2,2,4,5- tetrafluoro-5- (trifluorometossi)-1,3-diossolan-4-yl]ossi}acetico (C6O4)
- cloro-perfluoropolietere carbossilato, MFS-N2 (ADV-N2)
- cloro-perfluoropolietere carbossilato, MFS-N3 (ADV-N3)
- cloro-perfluoropolietere carbossilato, MFS-N4 (ADV-N4)
- cloro-perfluoropolietere carbossilato, MFS-N5 (ADV-N5)
- cloro-perfluoropolietere carbossilato, MFS-M3 (ADV-M3)
- cloro-perfluoropolietere carbossilato, MFS-M4 (ADV-M4)

DECRETO LEGISLATIVO 19 giugno 2025, n. 102.

# Quali PFAS supplementari? Come li selezionano?



PRECURSORE primario  
raw materials + commercial products

PRECURSORE secondario  
Degradation intermediates

RILASCIANO

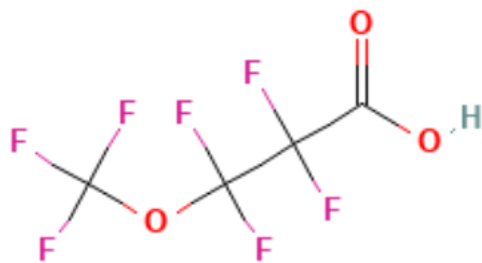
PFAA

Altri PFAS

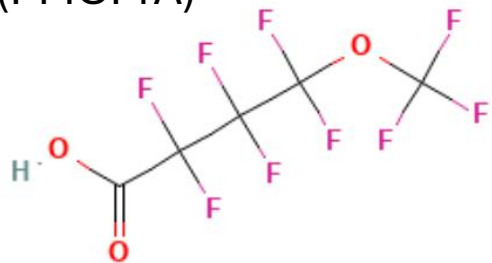
OSSIDAZIONE

PFAA  
+  
PFAA derivati  
dai precursori  
+  
Altri PFAS non  
precursori

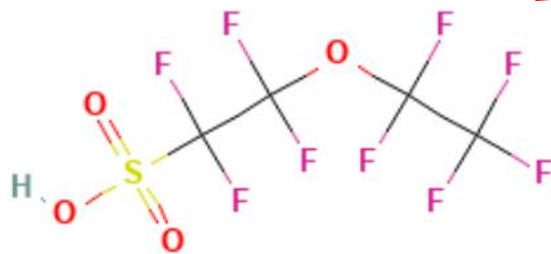
**PFAA**



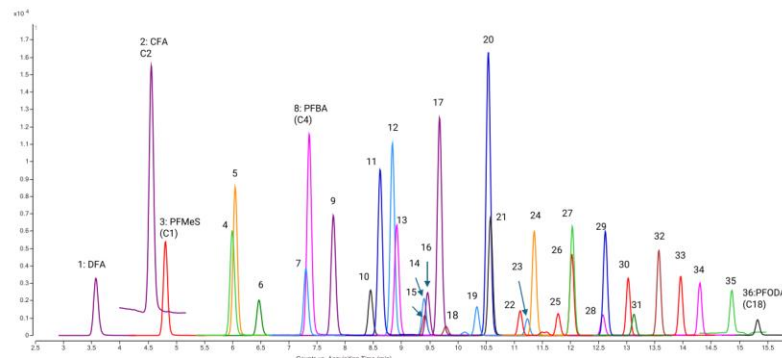
Perfluoro-3-methoxypropanoic acid (PMOPrA)



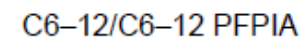
Perfluoro-4-methoxybutanoic acid  
PMOBA



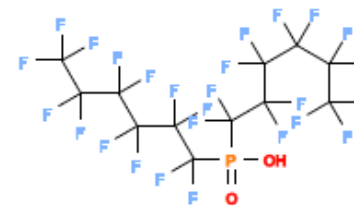
## Perfluoro(2-ethoxyethane)sulfonic acid (PFEESA)



- PFCA
- PFSA
- PFPA and PFPIA
- PFECA, PFESA

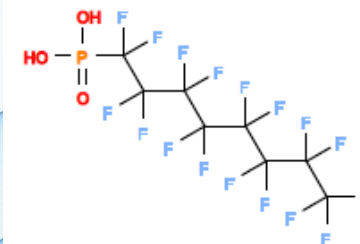


bis(perfluoroalkyl) (C6–C12) phosphinic acid



C6-12 PFPA

perfluoroalkyl (C6–C12) phosphonic acid



# Precursori: PAP e diPAP

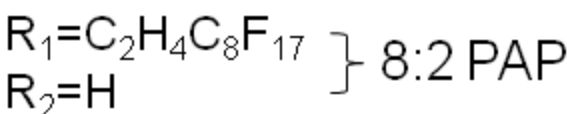
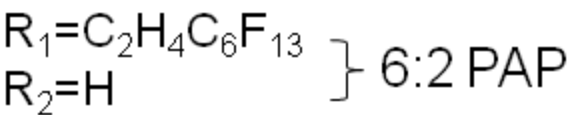
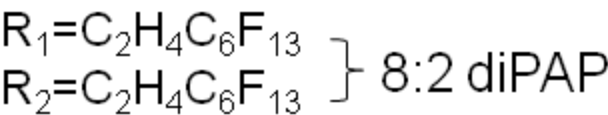
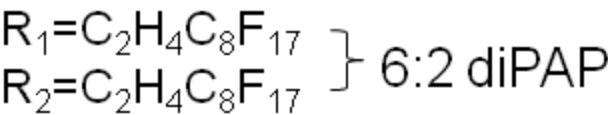
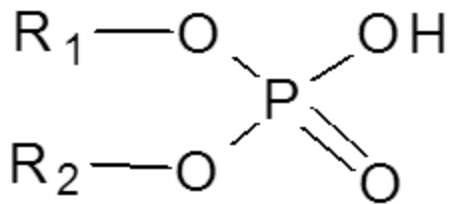
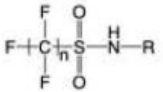
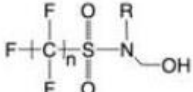
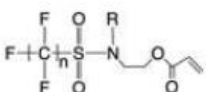
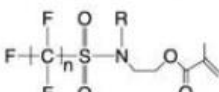
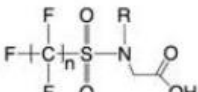
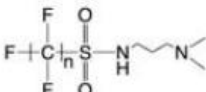
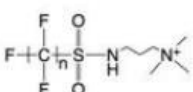
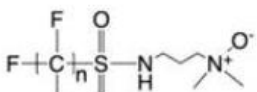
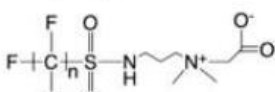


Table 4. Concentrations (ng/L) of polyfluoroalkyl phosphates (PAPs) detected in water plants of China.

| Compound       | Concentrations (ng/L) [mean ±RSD (%), n=3] |          |           |           |         |         |
|----------------|--------------------------------------------|----------|-----------|-----------|---------|---------|
|                | Beijing                                    | Haerbin  |           | Haikou    |         |         |
|                | Plant 1                                    | Plant 2  | Plant 3   | Plant 4   | Plant 5 | Plant 6 |
| 4:2 monoPAP    | – <sup>a</sup>                             |          |           |           |         | –       |
| 6:2 monoPAP    | –                                          |          | 13.0±1.4  |           |         | –       |
| 8:2 monoPAP    | –                                          |          | 3.6±1.5   |           |         | –       |
| 10:1 monoPAP   | 70.3±1.8                                   | 10.0±1.3 | 7.2±0.4   | 7.2±2.1   |         | 4.3±1.1 |
| 10:2 monoPAP   | 5.6±1.3                                    | 1.8±0.7  |           | 3.0±0.9   | 1.4±1.1 | –       |
| 4:2 diPAP      | –                                          |          |           |           |         | –       |
| 4:2/6:2 diPAP  | –                                          |          |           |           |         | –       |
| 6:2 diPAP      | –                                          |          |           |           |         | –       |
| 6:2/8:2 diPAP  | –                                          |          |           |           |         | –       |
| 8:2 diPAP      | –                                          |          | 0.10±0.05 | 0.10±0.05 |         | –       |
| 8:2/10:2 diPAP | –                                          |          |           |           |         | –       |
| 10:1 diPAP     | 0.8±1.2                                    |          | 1.4±0.7   | 3.8±1.6   |         | 1.5±1.0 |
| 10:2 diPAP     | –                                          |          |           |           |         | –       |
| Total          | 76.7                                       | 11.8     | 25.3      | 14.1      | 1.4     | 5.8     |

# Precursor: Perfluoroalkane sulfonamides and their derivatives (FASA)

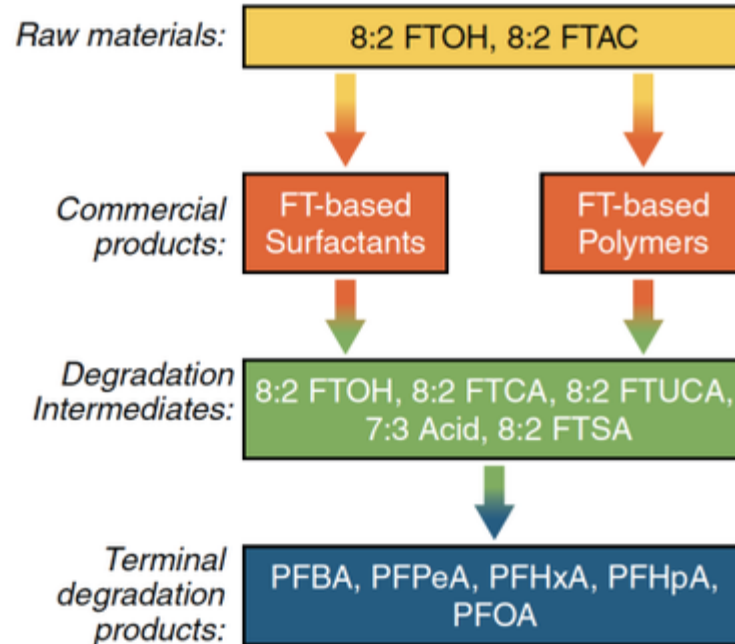
| Subclass                                                                                              | Chemical structure                                                                   | Chemical name                                                                                                                       | Use                                                               |
|-------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|
| <i>The blue 'A' represents alkyl length. For n = 4, 6, 8, A = B (butane), Hx (hexane), O (octane)</i> |                                                                                      |                                                                                                                                     |                                                                   |
| 1                                                                                                     |    | where R=H,<br>Perfluoroalkyl sulfonamides (FASA)<br>R=alkyl (methyl, ethyl),<br>N-alkyl FASA (MeFASA, EtFASA)                       | Major raw material for surfactant and surface protection products |
| 2                                                                                                     |    | where R=H,<br>Perfluoroalkane sulfonamidoethanols (FASE)<br>R=alkyl (methyl, ethyl),<br>N-alkyl FASE (MeFASE, EtFASE)               | Major raw material for surfactant and surface protection products |
| 3                                                                                                     |    | Where R=alkyl (methyl, ethyl),<br>N-Alkyl perfluoroalkane sulfonamidoethyl acrylates (FASAC)                                        | Major raw material for surfactant and surface protection products |
| 4                                                                                                     |    | Where R=alkyl (methyl, ethyl),<br>N-Alkyl perfluoroalkane sulfonamidoethyl methacrylates (FASMAC)                                   | Major raw material for surfactant and surface protection products |
| 5                                                                                                     |    | where R=H,<br>Perfluoroalkane sulfonamidoacetic acids (FASAA)<br>Where R=alkyl (methyl, ethyl),<br>N-alkyl FASAA (MeFASAA, EtFASAA) | Intermediate environmental transformation product                 |
| 6                                                                                                     |   | N-dimethyl ammonio propyl Perfluoroalkane sulfonamide (AmPr-FASA),<br>also referred to as PFASAm                                    | Functioning surfactants in AFFF-formulations                      |
| 7                                                                                                     |  | N-trimethyl ammonio propyl Perfluoroalkane sulfonamide (TAmPr-FASA),<br>also referred to as PFASAmS                                 | Functioning surfactants in AFFF-formulations                      |
| 8                                                                                                     |  | Perfluoroalkane sulfonamido amine oxides (PFASNO)                                                                                   | Functioning surfactants in AFFF-formulations                      |
| 9                                                                                                     |  | Perfluoroalkane sulfonamido betaine (PFASB)                                                                                         | Functioning surfactants in AFFF-formulations                      |

# Precursori

- PAP e diPAP, Polyfluoroalkyl phosphates
- FASA Perfluoroalkane sulfonamides
- FTSA, Fluorotelomer sulfonic acids
- FTCA, Fluorotelomer carboxylic acids

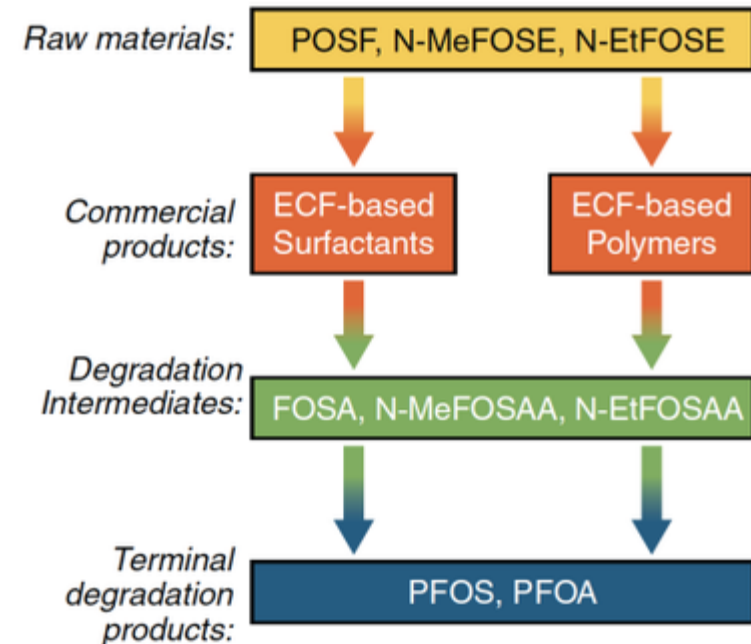
## Fluorotelomer Degradation Pathway Overview

*Example for 8:2 fluorotelomer homologue*



## ECF Degradation Pathway Overview

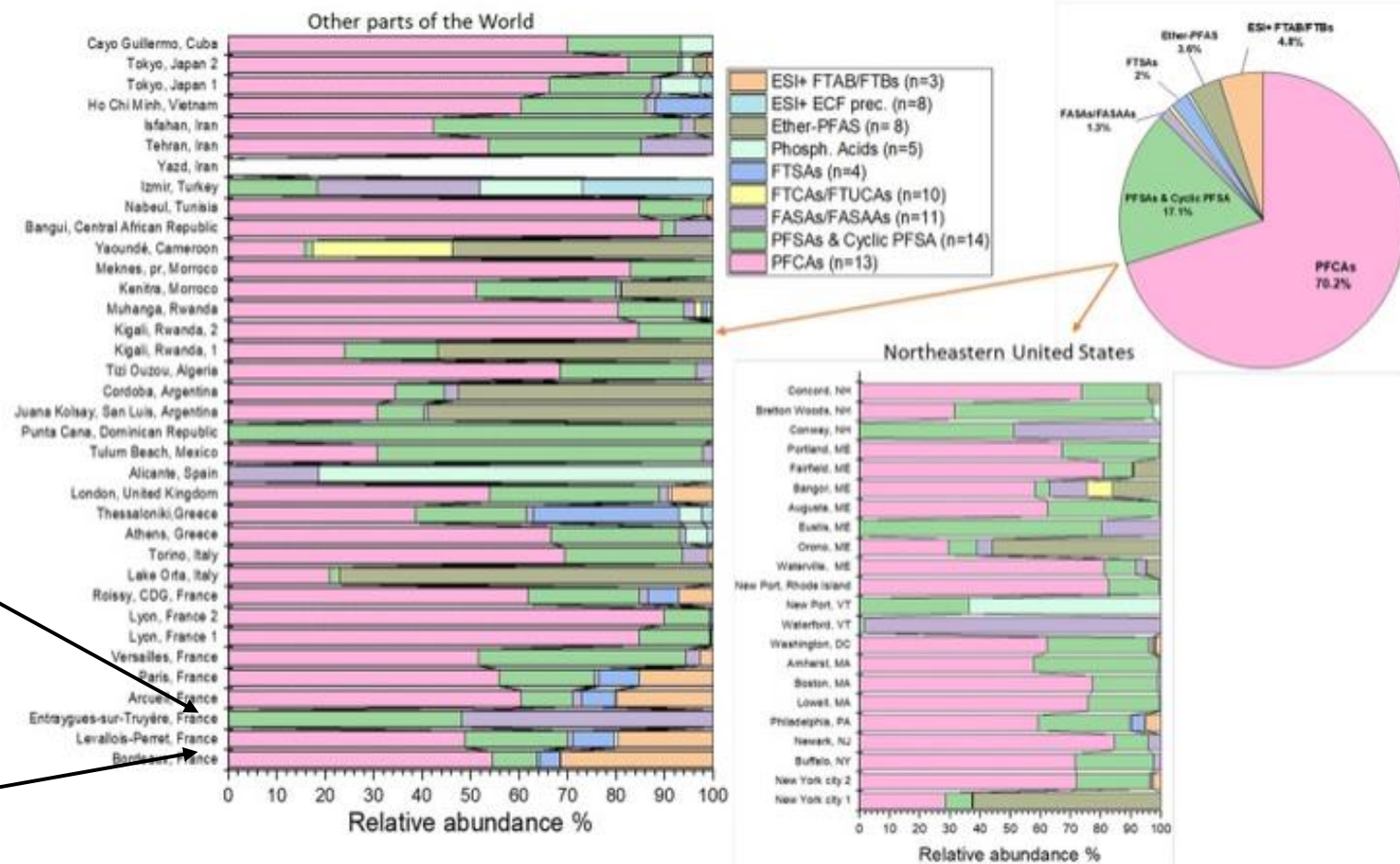
*Example for perfluorooctane sulfonyl homologue*



# Target Analysis Drinking water

50% FASA  
50% PFSA

30% FTAB/FTB  
10% FTS



Download: [Download high-res image \(737KB\)](#)

Download: [Download full-size image](#)

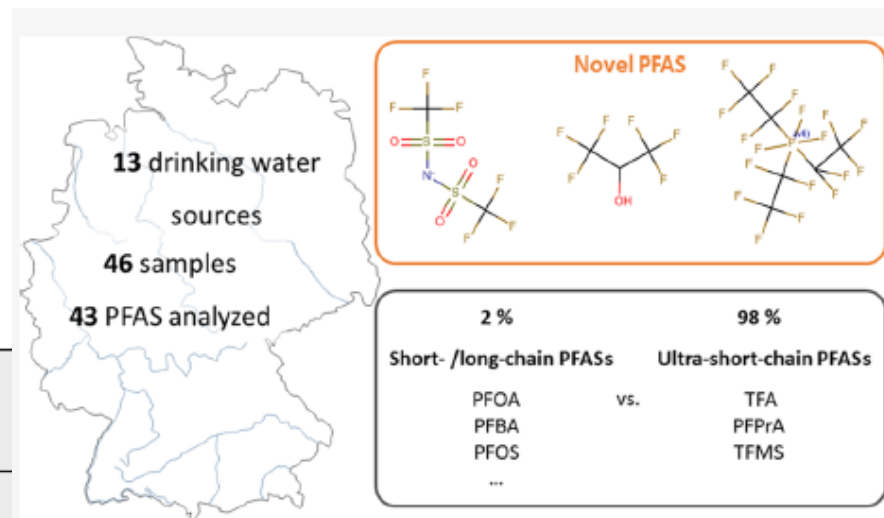
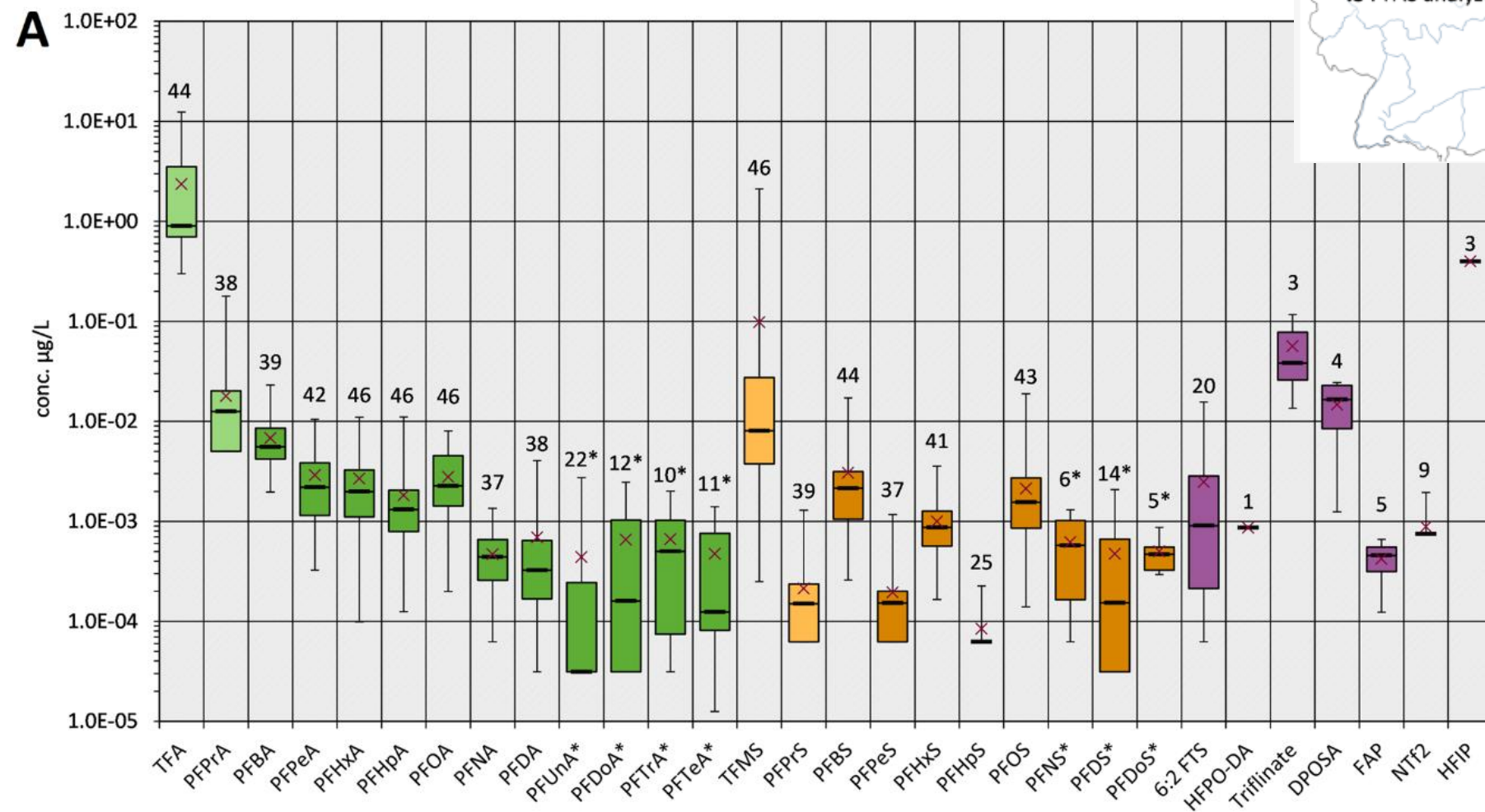
Fig. 5. Abundance and contribution of PFAS, subdivided by different groups in collected tap water samples from Northeastern USA and other parts of the world.

# Non precursori: ultrashort PFAS

| Name                                                       | Abbreviation | CAS_No      |
|------------------------------------------------------------|--------------|-------------|
| Trifluoroacetic acid                                       | TFA          | 76-05-1     |
| Perfluoropropanoic acid                                    | PFPrA        | 422-64-0    |
| Trifluoromethane sulfonic acid                             | TFMS         | 1493-13-6   |
| Perfluoroethane sulfonic acid                              | PFEtS        | 354-88-1    |
| Perfluoropropane sulfonic acid                             | PFPrS        | 423-41-6    |
| Perfluoro-2-methoxyacetic acid                             | PFMOAA       | 674-13-5    |
| Trifluoroacetamide                                         | TFAm         | 354-38-1    |
| Trifluoromethanesulfinic acid                              | TFSH         | 34642-42-7  |
| 1,1,2-Trifluoro-2-(trifluoromethoxy)ethane-1-sulfonic acid | 1:2 H-PFESA  | 905363-45-3 |
| 2,2,2-trifluoroethanol                                     | 1:1 FTOH     | 75-89-8     |
| 2,2-difluoropropan-1-ol                                    |              | 33420-52-9  |
| 3,3,3-trifluoropropan-1-ol                                 | 1:2 FTOH     | 2240-88-2   |
| 2,2,3,3,3-pentafluoropropan-1-ol                           | 2:1 FTOH     | 422-05-9    |
| Hexafluoroisopropanol                                      | HFiP         | 920-66-1    |

| Name                                                               | Abbreviation | CAS_No      |
|--------------------------------------------------------------------|--------------|-------------|
| <b>IONIC LIQUID</b>                                                |              |             |
| Bis(trifluoromethane)sulfonimide                                   | NTf2         | 82113-65-3  |
| Bis(perfluoroethylsulfonyl)imide                                   | BETI         |             |
| 1,1,2,2,2-Pentafluoroethylsulfonyl(trifluoromethylsulfonyl)azanide | FTNTf2       |             |
| N-(trifluoromethylsulfonyl) sulfamoyl fluoride                     | FTFSI        | 32819-50-4  |
| bis(fluorosulfonyl)imide                                           | FSI          | 14984-73-7  |
| Tris(pentafluoroethyl)trifluorophosphate                           | FAP          | 429679-87-8 |
| Heptafluoropropyltrifluorobate                                     |              |             |
| <b>INORGANIC FLUORIDE</b>                                          |              |             |
| sulfur hexafluoride                                                |              | 2551-62-4   |
| hexafluorophosphate                                                |              | 16919-18-9  |
| Hexafluoroarsenate                                                 |              |             |
| Boron trifluoride                                                  |              | 7637-07-2   |
| Tetrafluoroborate                                                  |              | 14874-70-5  |

# Ultrashort PFAS



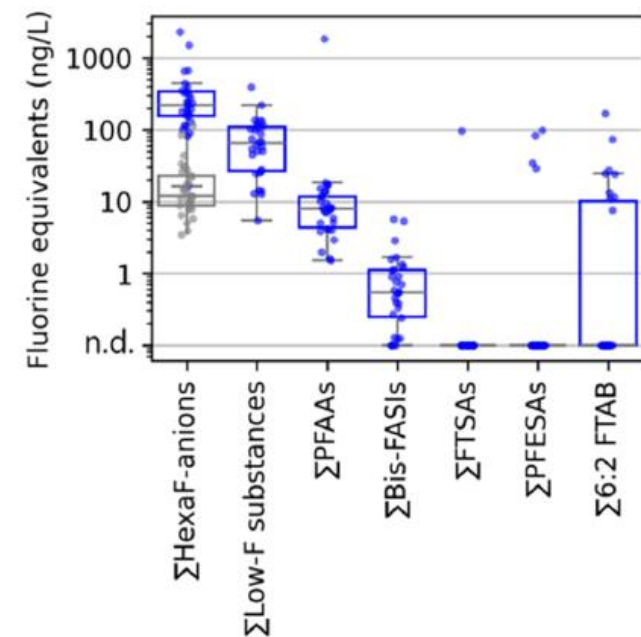
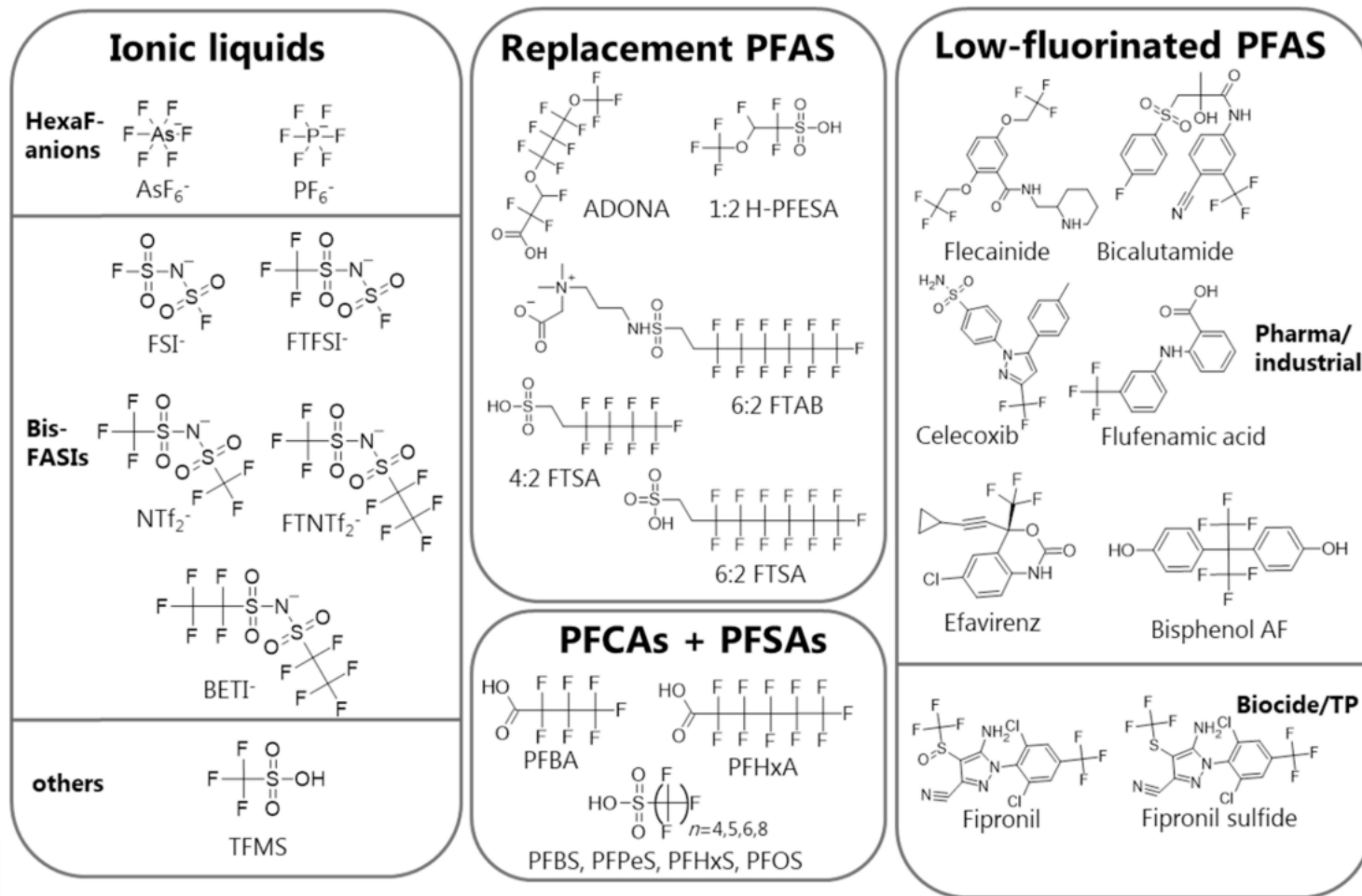
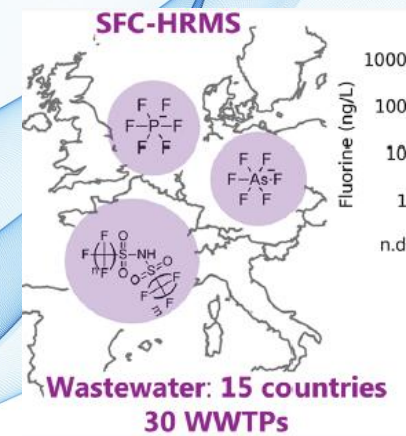


Figure 6. Fluorine equivalents calculated from the molecular formulas of identified and quantified compounds from wastewater effluent ( $n = 32$ ). PFAA = PFSAAs + PFCAs.  $\text{PF}_6^-$  concentrations were corrected for



# Suspect Screening (SS) e Non-Targeted Analysis (NTA) in HRMS

Journal of Exposure Science & Environmental Epidemiology

[www.nature.com/jes](http://www.nature.com/jes)

## ARTICLE



## Practical application guide for the discovery of novel PFAS in environmental samples using high resolution mass spectrometry

Mark Strynar<sup>1</sup> , James McCord<sup>1</sup>, Seth Newton<sup>1</sup>, John Washington<sup>1</sup>, Krista Barzen-Hanson<sup>2</sup>, Xenia Trier<sup>3</sup>, Yanna Liu<sup>4</sup>, Ian Ken Dimzon<sup>5</sup>, Boris Bugsel<sup>6</sup>, Christian Zwiener<sup>6</sup> and Gabriel Munoz<sup>7</sup>

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**Toolkit ENTAiLS** (<https://mccord-dev.github.io/ENTAiLSToolkit/#content>), USEPA

una raccolta delle migliori pratiche e un flusso di lavoro open-source per l'elaborazione dei dati destinati agli studi di NTA (Non-Targeted Analysis) sui PFAS. Comprende linee guida + strumenti integrati per l'identificazione e la caratterizzazione dei PFAS nelle risorse idriche potabili.

[10.1007/s00216-025-05921-0](https://doi.org/10.1007/s00216-025-05921-0)

# SS e NTA in HRMS: Mass Lists and Mass Spectral Database



Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

NORMAN Suspect List Exchange – NORMAN SLE

 **MassBank**  
High Quality Mass Spectral Database

**NIST** PUBLIC  
DATA REPOSITORY 1.8.0

Public Data Resource

Suspect List of Possible Per- and Polyfluoroalkyl Substances (PFAS)



Environmental Topics

Laws & Regulations

CompTox Chemicals Dashboard

Home



Advanced Mass Spectral Database

# SS e NTA (PFAS)

- intervallo caratteristico dei difetti di Massa (n -0.1 and +0.15 Da)
- Unità ripetute ricorrenti (Kendrick mass defect)
- Frammenti diagnostici

**Table 2.** Common fragments, losses and adducts of PFAS in the ESI<sup>-</sup> mode.

| Fragment                                                                                                                                   | Mass (Da)                   | Losses                         | Mass (Da)                 |
|--------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|--------------------------------|---------------------------|
| CF <sub>3</sub> <sup>-</sup> , C <sub>2</sub> F <sub>5</sub> <sup>-</sup> , C <sub>3</sub> F <sub>7</sub> <sup>-</sup>                     | 68.9952, 118.9920, 168.9888 | CO <sub>2</sub>                | 43.9898                   |
| CF <sub>3</sub> O <sup>-</sup> , C <sub>2</sub> F <sub>5</sub> O <sup>-</sup> , C <sub>3</sub> F <sub>7</sub> O <sup>-</sup>               | 84.9901, 134.9869, 184.9837 | SO <sub>3</sub>                | 79.9568                   |
| C <sub>2</sub> F <sub>3</sub> <sup>-</sup> , C <sub>3</sub> F <sub>5</sub> <sup>-</sup> , C <sub>4</sub> F <sub>7</sub> <sup>-</sup>       | 80.9952, 130.9920, 180.9888 | H <sub>2</sub> CO              | 30.0106                   |
| C <sub>2</sub> F <sub>3</sub> O <sup>-</sup> , C <sub>3</sub> F <sub>5</sub> O <sup>-</sup> , C <sub>4</sub> F <sub>7</sub> O <sup>-</sup> | 96.9901, 146.9869, 196.9837 | CO                             | 27.9949                   |
| CF <sub>2</sub> O <sup>-</sup> , C <sub>2</sub> F <sub>4</sub> O <sup>-</sup> , C <sub>3</sub> F <sub>6</sub> O <sup>-</sup>               | 65.9917, 115.9885, 165.9853 | HF                             | 20.0062                   |
| C <sub>2</sub> F <sub>4</sub> <sup>-</sup> , C <sub>2</sub> F <sub>4</sub> <sup>-</sup> , C <sub>3</sub> F <sub>6</sub> <sup>-</sup>       | 99.9936, 149.9904, 199.9872 | FSO <sub>3</sub>               | 98.9552                   |
| C <sub>3</sub> F <sub>6</sub> ClO <sup>-</sup>                                                                                             | 200.9542                    | H <sub>3</sub> PO <sub>4</sub> | 97.9769                   |
| SO <sub>2</sub> F <sup>-</sup> , SO <sub>3</sub> F <sup>-</sup>                                                                            | 82.9603, 98.9552            | <b>Adducts and n-mers</b>      | <b>Δ Mass (Da) from M</b> |
| C <sub>2</sub> F <sub>4</sub> SO <sub>3</sub> <sup>-</sup>                                                                                 | 179.9504                    | [M - H + Na] <sup>-</sup>      | 21.981945                 |
| C <sub>2</sub> F <sub>5</sub> N <sup>-</sup>                                                                                               | 132.9951                    | [2M + H] <sup>-</sup>          | M + 1.007825              |
|                                                                                                                                            |                             | [2M + Na] <sup>-</sup>         | M + 21.981945             |

The accurate mass is a summation of all composition elements while neglecting the electron (0.00054858 Da). **M** refers to the negatively charged molecular ion, and **Δ Mass** refers to the mass deviation from M.

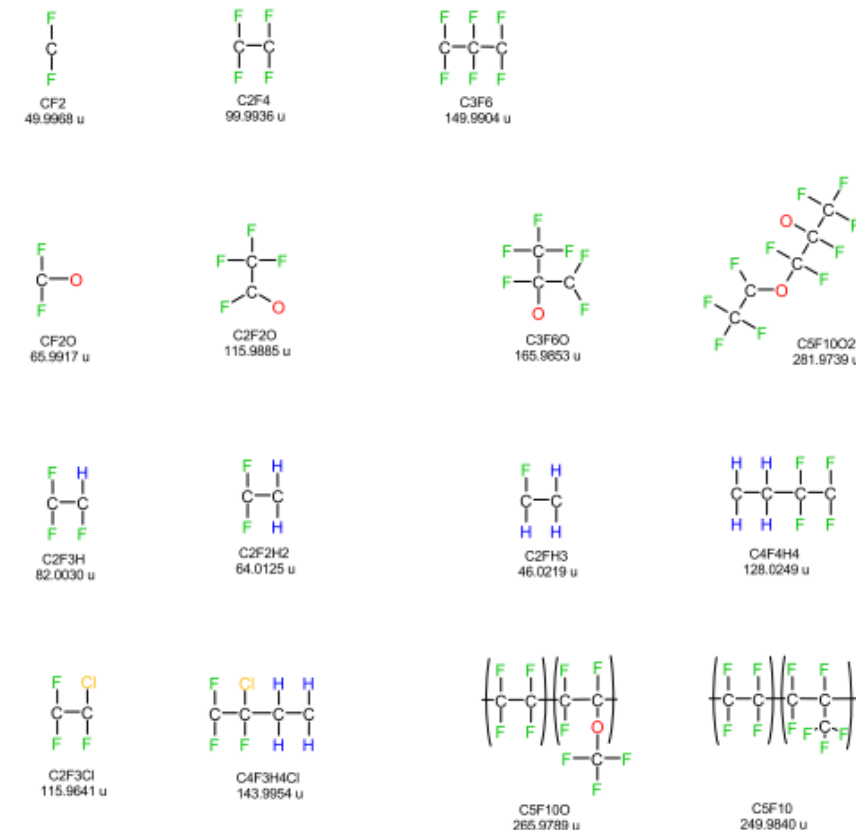
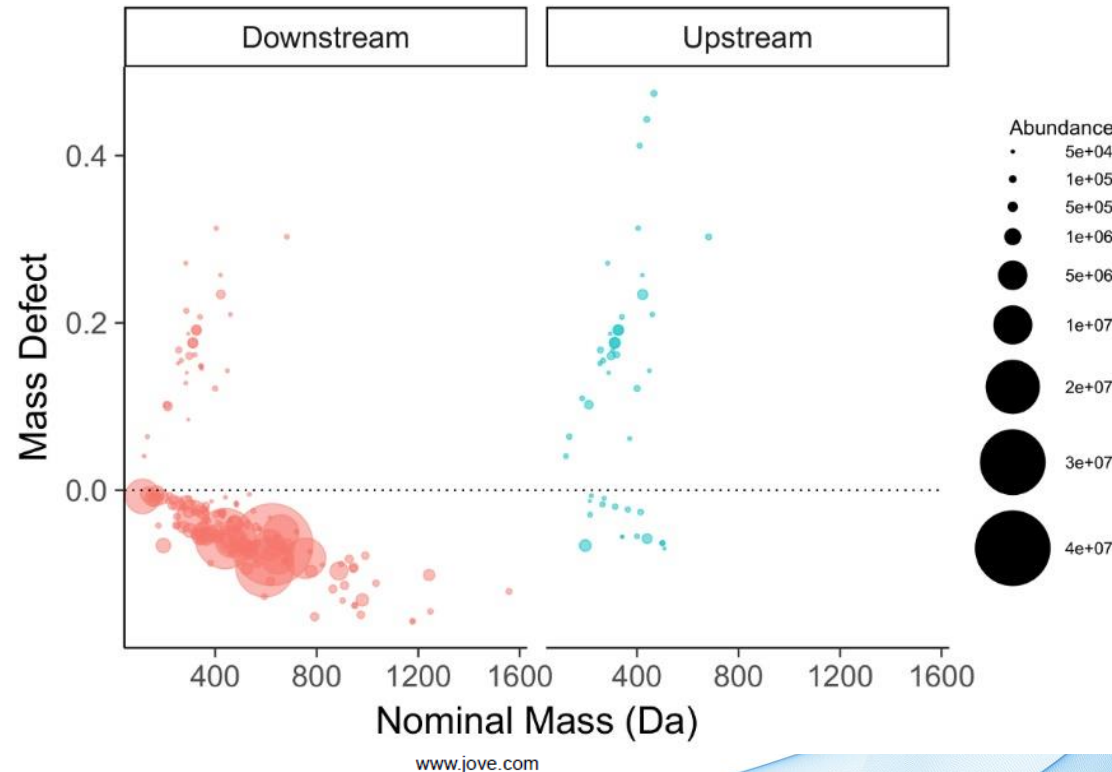


**Fig. 2** Common PFAS repeating units.

**FluoroMatch** è una suite di software open-source e vendor-neutral progettata per l'analisi e l'annotazione automatizzata di sostanze per- e polifluoroalchiliche (PFAS) in campioni complessi tramite spettrometria di massa ad alta risoluzione (HRMS). [[10.1007/s00216-021-03392-7](https://doi.org/10.1007/s00216-021-03392-7)]

# SS e NTA in HRMS: Uso dei *mass defect* delle serie di unità $\text{CF}_2$

Grafico dei difetti di massa per le caratteristiche chimiche identificate in un fiume a valle (rosso, a sinistra) e a monte (blu, a destra) di uno scarico un sito di produzione fluorochimica



**jove** Journal of Visualized Experiments

Video Article

**Identifying Per- and Polyfluorinated Chemical Species with a Combined Targeted and Non-Targeted-Screening High-Resolution Mass Spectrometry Workflow**

James McCord<sup>1</sup>, Mark Strynar<sup>2</sup>

# SS e NTA in HRMS: Uso dei frammenti diagnostici per PFAS

analytical  
chemistry

Article

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Discovery of  $C_5$ – $C_{17}$  Poly- and Perfluoroalkyl Substances in Water by In-Line SPE-HPLC-Orbitrap with In-Source Fragmentation Flagging

Yanna Liu, Alberto Dos Santos Pereira,<sup>†</sup> and Jonathan W. Martin\*

36 nuovi PFAS in  
effluente di WWTP

Environmental  
Science & Technology

Article

Cite This: Environ. Sci. Technol. 2018, 52, 5830–5840

pubs.acs.org/est

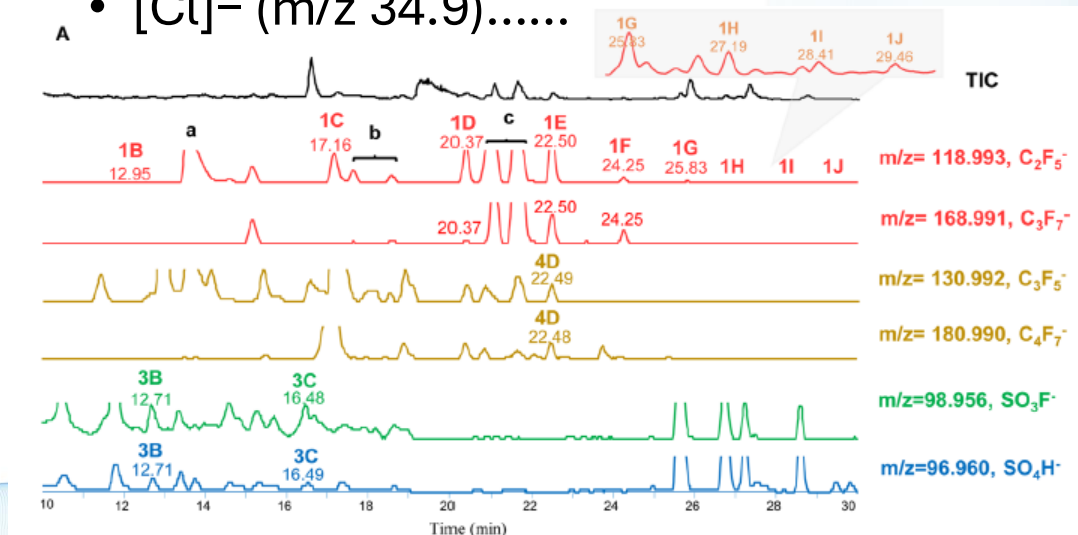
Nontarget Mass Spectrometry Reveals New Perfluoroalkyl Substances in Fish from the Yangtze River and Tangxun Lake, China

Yanna Liu,<sup>†</sup> Manli Qian,<sup>‡</sup> Xinxin Ma,<sup>§</sup> Lingyan Zhu,<sup>§</sup> and Jonathan W. Martin<sup>\*,†,||</sup>

330 nuovi PFAS (di 4 nuove  
classi di PFAS) nel fegato di  
pesci

in-source fragmentation flagging  
scans:

- $[C_2F_5]^-$  ( $m/z$  118.992)
- $[C_3F_7]^-$  ( $m/z$  168.988)
- $[SO_4H]^-$  ( $m/z$  96.959)
- $[Cl]^-$  ( $m/z$  34.9).....



# Sfide analitiche per i PFAS: Non Target Screening (NTS) in HRMS: Uso dei *mass defect* delle serie di unità $\text{CF}_2$

Analytical and Bioanalytical Chemistry (2020) 412:4797–4805  
<https://doi.org/10.1007/s00216-019-02358-0>

PAPER IN FOREFRONT

LC-MS screening of poly- and perfluoroalkyl substances  
in contaminated soil by Kendrick mass analysis

Boris Bugsel<sup>1</sup> · Christian Zwiener<sup>1</sup> 

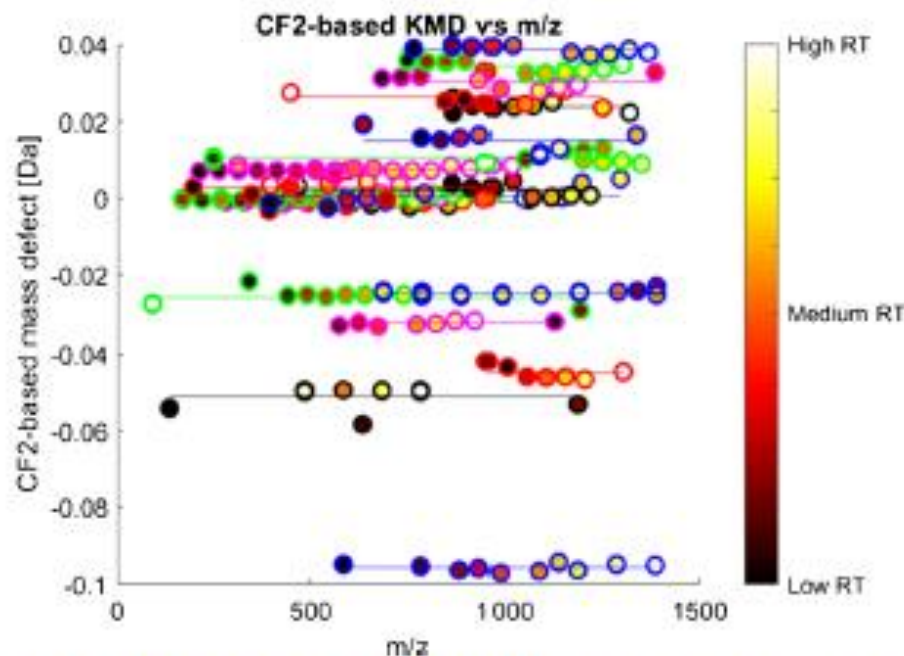


**Fig. 1** Kendrick mass defect for  $\text{CF}_2$  repeating units vs. mass-to-charge ratio. Only selected HS with at least 7 homologues are shown. Each feature is represented by a circle in different colors to distinguish HS.

Riconoscimento in serie di composti omologhi attraverso l'uso di grafici dei difetti di massa di Kendrick

La serie omologa è una serie di composti con lo stesso gruppo funzionale e proprietà simili in cui i membri della serie differiscono per il numero di unità ripetitive che contengono (es. **PFAS**  $(\text{F}-(\text{CF}_2)_n\text{-X})$ )

Kendrick Mass (KM) =  $m/z \cdot (\text{Nominal (round)} M_{\text{unit}} / M_{\text{unit}})$   
KMD (Kendrick Mass Defect) =  $\text{Nominal (round)} \text{KM} - (\text{KM})$



**Grazie per l'attenzione**